

# Asymmetric magnetic interference patterns in $0-\pi$ Josephson junctions.

D.F. Agterberg<sup>1</sup> and M. Sigrist<sup>1,2</sup>

<sup>1</sup> *Theoretische Physik, ETH- Hönggerberg, 8093 Zürich, Switzerland*

<sup>2</sup> *Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-01, Japan*

(February 1, 2008)

We examine the magnetic interference patterns of Josephson junctions with a region of  $0$ - and of  $\pi$ -phase shift. Such junctions have recently been realized as  $c$ -axis YBCO-Pb junctions with a single twin boundary in YBCO. We show that in general the junction generates self-fields which introduces an asymmetry in the critical current under reversal of the magnetic field. Numerical calculations of these asymmetries indicate that they account well for unexplained features observed in single twin boundary junctions.

74.20.Mn, 74.25.Bt

Josephson tunneling experiments on the high temperature superconducting compound  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) have played an important role in establishing the predominantly  $d$ -wave symmetry of the superconducting order parameter [1–8]. However, YBCO has orthorhombic symmetry which implies that the order parameter cannot be purely  $d$ -wave and must contain an additional  $s$ -wave contribution [9–13]. This has significant consequences for  $c$ -axis Josephson tunneling experiments between YBCO and Pb (a standard  $s$ -wave superconductor). In such junctions the  $d$ -wave component is forbidden by symmetry to contribute to the lowest order Josephson current so that the observed current [9] is due solely to the  $s$ -wave component of the YBCO. There is a clear difference between untwinned and twinned YBCO samples in the observed current. The current is considerably suppressed for the latter compared to that of the former. This can be understood if we assume that the  $d$ -wave component is essentially uniform while the  $s$ -wave component changes sign at each twin boundary, *i.e.* a twinned sample yields a  $c$ -axis junction with alternating  $0$ - and  $\pi$ -phase shift regions. This alternation of sign (or phase) gives rise to destructive interference effects for the total Josephson current in heavily twinned samples [10].

To gain more insight into the  $c$ -axis Josephson tunneling results Kouznetsov *et. al.* [14] have built  $c$ -axis YBCO - Pb junctions that contain a single twin boundary and have measured its magnetic interference pattern. These elegant experiments show that the critical current as a function of the applied magnetic field,  $I_c(\mathbf{H}_e)$ , behaves qualitatively like a junction separated into two regions, one with  $0$ - and the other with  $\pi$ -phase shift (such a model naturally arises due to  $\pi$  phase change of the  $s$ -wave component as the twin boundary is crossed). A noteworthy unexplained feature of the data in Ref. [14] is an asymmetry between  $I_c(\mathbf{H}_e)$  and  $I_c(-\mathbf{H}_e)$  for fields in the junction plane that are neither along the twin boundary nor orthogonal to it. In the short junction limit (for which the junction dimensions are much smaller than the

Josephson penetration depth) such an asymmetry implies that time reversal symmetry is broken in the junction when there are no applied currents or magnetic fields [15]. For example such an asymmetry will occur if there is local broken time reversal symmetry due to a phase difference of  $\pi/2$  between the  $s$  and  $d$  components at the twin boundary (far from the twin boundary this phase difference must be  $0$  or  $\pi$ ) [15,14].

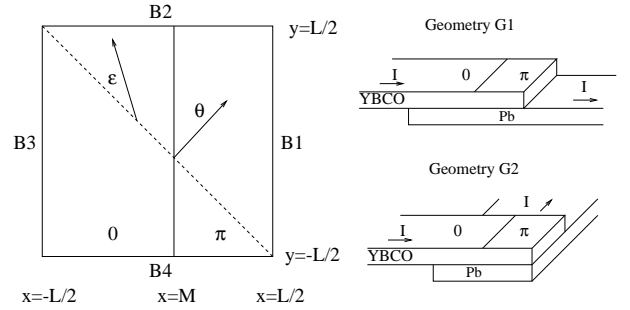


FIG. 1. Junction geometries considered in this article. The left figure shows the junction plane while the right figures depict the two geometries considered in this article.

In this article we present another origin for such an asymmetry in junctions that are time reversal invariant. In particular, such asymmetries arise whenever parity symmetry is broken in these junctions. This parity breaking can occur in two ways: either the junction is not invariant under a parity transformation about the center of the junction (intrinsic parity breaking) or the current running from the leads into the junction does not obey  $I|_{\partial S} = I|_{-\partial S}$  where  $\partial S$  is the boundary of the junction (*e.g* the current does not enter and leave a rectangular junction through opposite edges) (extrinsic parity breaking). In the context of the  $0-\pi$  junction model for a single twin boundary the junction has intrinsic parity symmetry whenever the twin boundary lies in the center of the junction (called a symmetric junction after Kirtley *et. al.* [16]). A numerical study for a symmetric  $0-\pi$  junction with extrinsic broken parity

symmetry is shown to account well for the experimentally observed magnetic diffraction patterns. Numerical studies of asymmetric  $0 - \pi$  junctions with extrinsic parity conserving boundary conditions also reveals asymmetries that should be observable in experiments like those of Ref. [14]. This discussion is also of relevance to corner junction flux modulation experiments [5,8,17].

We consider here junctions with the two geometries shown in Fig.1. The geometry *G2* breaks extrinsic parity symmetry while *G1* does not. The coordinates perpendicular and parallel to the twin boundary are called  $x$  and  $y$ , respectively. The order parameter of the Pb has standard  $s$ -wave symmetry,  $\Psi_{Pb} = |\Psi_{Pb}|e^{i\varphi}$ . For YBCO there are two components  $(\Psi_d, \Psi_s) = e^{i\varphi'}(|\Psi_d|, e^{i\alpha}|\Psi_s|)$  where  $\Psi_d$  and  $\Psi_s$  correspond to the  $d$ - and  $s$ -wave components, respectively. The relative phase  $\alpha$  is fixed by the bulk free energy of YBCO and is 0 for one type of twin domain and  $\pi$  for the other [10,11]. The intrinsic phase shift of the junction is determined by  $\alpha$ . Note that the choice of  $\alpha$  equal to 0 or  $\pi$  is a matter of convention (freedom of gauge in the two superconductors). However, once it is fixed somewhere in the junction it is determined everywhere.

The Josephson phase, the local phase difference  $\phi = \varphi - \varphi'$  over the junction follows the relation  $\mathbf{H}(\mathbf{x}) \times \hat{z} = (\Phi_0/2\pi\tilde{d})(\nabla\phi)$  while  $\mathbf{H}$  satisfies the Maxwell equation  $\nabla \times \mathbf{H} = 4\pi\mathbf{j}/c$  ( $\Phi_0 = hc/2e$ ) [18]. For the lowest order Josephson coupling (between  $\Psi_s$  and  $\Psi_{Pb}$ ) we can express  $j_z$  as  $j_c(\mathbf{x}) \sin[\phi + \alpha(\mathbf{x})]$  ( $j_c(\mathbf{x}) > 0$ ). By restricting  $\alpha(\mathbf{x})$  to take on the values 0 or  $\pi$  and allowing  $j_c(\mathbf{x})$  to take on any value this relation for  $j_z$  describes any time reversal invariant junction. We therefore use this form for more general considerations and then specify  $j_c(\mathbf{x})$  and  $\alpha(\mathbf{x})$  to describe the  $0 - \pi$  model for the single twin boundary junction for numerical results. Together these relations lead to the Sine-Gordon equation describing the spatial dependence of  $\phi$  throughout the bulk of the junction [10,11,18].

$$\nabla^2 \phi = \lambda_J^{-2}(\mathbf{x}) \sin[\phi + \alpha(\mathbf{x})], \quad (1)$$

where  $\lambda_J(\mathbf{x}) = [\Phi_0/2\pi\tilde{d}j_c(\mathbf{x})]^{1/2}$  with the boundary conditions

$$\bar{\lambda}_J \mathbf{n} \cdot \nabla \phi|_{\partial S} = \mathbf{n} \cdot (\mathbf{h} \times \hat{z})|_{\partial S} \quad (2)$$

where  $\mathbf{n}$  is the outward normal to the boundary  $\partial S$ . The variable  $\mathbf{h}$  is a function of the reduced variables  $\mathbf{h}^e = \frac{2ed\lambda_J}{\hbar c} \mathbf{H}_e$  ( $\mathbf{H}_e$  is the applied external field) and  $i = \frac{I}{2\lambda_J L \bar{j}_c}$  where  $\bar{j}_c$  is the average value of  $j_c(\mathbf{x})$  and  $\bar{\lambda}_J$  is determined from  $\bar{j}_c$ . For the geometries shown in Fig 1 Ampere's Law implies [19] that we have for G1 (extrinsic parity conserving boundary conditions)

$$\mathbf{n} \cdot [\mathbf{h} \times \hat{z}]|_{\partial S} = \begin{cases} h_y^e + i & \partial S = B1 \\ -h_x^e & \partial S = B2 \\ -h_y^e + i & \partial S = B3 \\ h_x^e & \partial S = B4. \end{cases} \quad (3)$$

and for G2 (extrinsic parity violating boundary conditions)

$$\mathbf{n} \cdot [\mathbf{h} \times \hat{z}]|_{\partial S} = \begin{cases} h_y^e & \partial S = B1 \\ -h_x^e + i & \partial S = B2 \\ -h_y^e + i & \partial S = B3 \\ h_x^e & \partial S = B4. \end{cases} \quad (4)$$

The Sine-Gordon equation and the boundary conditions can be recast into a variational form with the functional

$$F = \bar{\lambda}_J \int_S d^2x \left[ (\nabla\phi)^2 / 2 - \lambda_J^{-2}(\mathbf{x}) \cos(\phi + \alpha(\mathbf{x})) \right] + \int_{\partial S} dx \phi [\mathbf{n} \cdot (\mathbf{h} \times \hat{z})]. \quad (5)$$

The positive and negative critical currents of the junction are defined as the maximal positive and negative supercurrents, respectively, that can pass through the junction. They satisfy the following symmetry relations based on the structure of  $F$ :

$$I_c[\mathbf{H}_e, \alpha(\mathbf{x}), \lambda_J(\mathbf{x})] = -I_c[-\mathbf{H}_e, -\alpha(\mathbf{x}), \lambda_J(\mathbf{x})] \quad (6)$$

$$I_c[\mathbf{H}_e, \alpha(\mathbf{x}), \lambda_J(\mathbf{x})] = I_c[\mathbf{H}_e, \alpha(\mathbf{x}) + \alpha_0, \lambda_J(\mathbf{x})] \quad (7)$$

where  $\alpha_0$  is a constant phase shift. Eqs. 6 and 7 follow from the time reversal and gauge invariance of the junction respectively. For geometry G1, due to the extrinsic parity symmetry, the following relation also holds

$$I_c[\mathbf{H}_e, \alpha(\mathbf{x}), \lambda_J(\mathbf{x})] = I_c[-\mathbf{H}_e, \alpha(-\mathbf{x}), \lambda_J(-\mathbf{x})] \quad (8)$$

more specifically this is a result of the invariance of  $F$  in Eq. (5) under the transformation  $\mathbf{h}^e \rightarrow -\mathbf{h}^e$ ,  $\alpha(\mathbf{x}) \rightarrow \alpha(-\mathbf{x})$ ,  $\lambda(\mathbf{x}) \rightarrow \lambda(-\mathbf{x})$ , and  $\phi(\mathbf{x}) \rightarrow \phi(-\mathbf{x})$  (a product of time reversal and parity symmetries). No such relation holds for geometry *G2* which has broken extrinsic parity breaking). If the junction is time reversal invariant then the phase  $\alpha(\mathbf{x})$  is restricted to be 0 or  $\pi$ . For such a junction  $I_c(\mathbf{H}_e) = I_c(-\mathbf{H}_e)$  is required if the boundaries have extrinsic parity symmetry, if  $j_c(\mathbf{x}) = j_c(-\mathbf{x})$ , and if  $\alpha(\mathbf{x}) = \alpha(-\mathbf{x})$  or if  $\alpha(\mathbf{x}) = \alpha(-\mathbf{x}) + \pi$ . Consequently the observation of  $I_c(\mathbf{H}_e) \neq I_c(-\mathbf{H}_e)$  in junctions that are time reversal invariant is due to broken parity symmetry in the junction. In the following we will consider the  $0 - \pi$  model for the single twin boundary junction where  $\lambda_J(\mathbf{x}) = \lambda_J$  and  $\alpha(\mathbf{x}) = \pi\Theta(x - M)$  where  $\Theta$  is the step function and  $-L/2 < M < +L/2$  ( $M$  is the position of the twin boundary according to Fig.1).

Consider the geometry G1. The one dimensional model that results when the magnetic field is applied along the twin boundary has been previously studied by several groups (e.g. see Ref. [16,17]). Using the relations (7) and (8) with  $\alpha_0 = \pi$  it is easy to see that  $I_c(\mathbf{H}_e) = I_c(-\mathbf{H}_e)$  if the twin boundary lies in the center of the junction (a symmetric junction [16]). For other positions of the twin boundary there is no symmetry constraint to enforce

$I_c(\mathbf{H}_e) \neq I_c(-\mathbf{H}_e)$ , however it can be shown for these asymmetric  $0 - \pi$  junctions that

$$I_c(h_x^e, h_y^e) = I_c(-h_x^e, h_y^e). \quad (9)$$

Numerical analysis shows  $I_c(\mathbf{H}_e) \neq I_c(-\mathbf{H}_e)$  when  $h_y^e \neq 0$  for asymmetric  $0 - \pi$  junctions (see below). As pointed out earlier [17] the change of  $\alpha$  from 0 to  $\pi$  introduces a spontaneous flux line corresponding to a “ $\pi$  vortex”, i.e. vortex of half the conventional phase winding and a flux  $\Phi_0/2$ , if the junction is much longer than the screening length  $\lambda_J$  [20]. Even for junctions with a length comparable to  $\lambda_J$  such self fields appear. However, in this case the screening is imperfect and new effects due to the position of the twin boundary arise. For an asymmetric junction the screening is more effective for the longer of the  $\alpha = 0$  or  $\alpha = \pi$  regions leading to  $I_c(\mathbf{H}_e) \neq I_c(-\mathbf{H}_e)$ . Note that the time reversal invariance of asymmetric  $0 - \pi$  junctions requires  $I_c(\mathbf{H}_e) = -I_c(-\mathbf{H}_e)$  so that experiments in which the positive and negative critical currents are averaged (such as in Ref. [8]) will not reveal this asymmetry. A recent careful numerical study of this model when the magnetic field is along the twin boundary by Kirtley *et. al.* [16] only considered one sign of the applied field and consequently did not uncover this asymmetry.

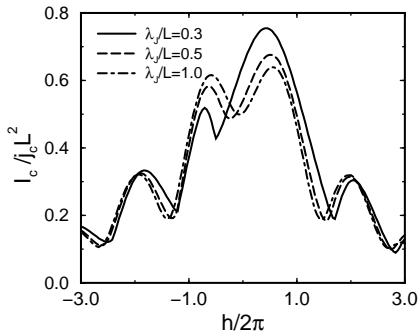


FIG. 2.  $I_c(H_e)/j_c L^2$  for geometry G1,  $M/L = 0.25$ , and  $\lambda_J/L = 0.3, 0.5$ , and  $1.0$  from top to bottom respectively.  $I_c(H_e)$  represents the positive critical current and the negative critical current is given by  $-I_c(-H_e)$ .

To examine the magnitude of the difference between  $I_c(\mathbf{H}_e)$  and  $I_c(-\mathbf{H}_e)$  for asymmetric  $0 - \pi$  junctions a numerical calculation is required. Since the two dimensional problem is numerically intensive a detailed study for the field along the twin boundary (for which the problem becomes one dimensional) was done. The technique we use is to discretize the variable  $\phi(x)$  into  $N$  variables and to minimize the free energy by a quasi-Newton technique. The critical current was found by increasing the current until no stable minimum can be found anymore. The criterion for failure to reach a stable state in  $F$  in Eq. 5 is similar to that used by

Kirtley *et. al.* [16] and is given by  $\epsilon > 10^{-4}$  where  $(\epsilon/\pi)^2 = [\phi_1 - \phi_2 - (i - h)/\alpha^{1/2}]^2 + [\phi_N - \phi_{N-1} - (i + h)/\alpha^{1/2}]^2 + \sum_{i=2}^{N-1} [\phi_{i+1} + \phi_{i-1} - 2\phi_i - \sin(\phi_i + \theta_i)/\alpha]^2$  where  $\alpha = N\lambda_J^2/L^2$ . Our numerical results using  $N = 100$  for the symmetric  $0 - \pi$  junction and for the  $0 - 0$  junction agree well with those found by Kirtley *et. al.* [16]. Fig. 2 shows the results for  $M/L = 1/4$  and for a variety of penetration depths. The asymmetry between  $I_c(H_e)$  and  $I_c(-H_e)$  is clearly visible and this further implies that zero field does not correspond to either a maximum or a minimum of the magnetic diffraction pattern.

Now consider the geometry G2. This geometry is the relevant one for the experiments on single twin boundary junctions [14] and in this case there are no symmetry relations enforcing  $I_c(\mathbf{H}_e) = I_c(-\mathbf{H}_e)$  for symmetric  $0 - \pi$  junctions due to extrinsic parity breaking. To gain an understanding of the effects of this geometry on the  $I_c(\mathbf{H}_e)$  pattern it is helpful to first consider  $0 - 0$  junctions (*i.e.*  $\lambda_J(\mathbf{x}) = \lambda_J$  and  $\alpha(\mathbf{x}) = 0$  independent of  $\mathbf{x}$ ). Symmetry relations enforce  $I_c(\mathbf{H}_e) = I_c(-\mathbf{H}_e)$  when the field is along the dotted diagonal shown in Fig. 1. These relations also imply  $I_c(H_e, \epsilon) = I_c(-H_e, -\epsilon)$  where  $\epsilon$  is defined in Fig. 1. A 2D generalization (for a 30 by 30 system and  $L/\lambda_J = 5$ ) of the 1D numerical method presented earlier shows that as expected a conventional  $I_c(\mathbf{H}_e)$  for  $\epsilon = 0$  arises and as  $\epsilon$  increases the central peak tilts so that the maximum  $I_c$  moves from  $H_e = 0$  to positive fields. The maximum  $I_c$  is furthest away from  $H_e = 0$  for  $\epsilon = \pi/2$ . We have not been able to find any experimental reports of this angular dependent  $I_c(\mathbf{H}_e)$  pattern for conventional Josephson junctions. To some degree this angular asymmetry still occurs for the  $0 - \pi$  junction. For the  $0 - \pi$  junction the interplay of the presence of the  $0 - \pi$  phase shift and the geometry makes a qualitative discussion difficult. In Fig. 3 we present numerical results on a 30 by 30 system for  $\lambda_J = 1/2$ . The numerical results exhibit all of the main features observed in experiments: the asymmetry is not apparent for the field along or perpendicular to the twin boundary but is so for other field orientations, the sign of  $I_c(\mathbf{H}_e) - I_c(-\mathbf{H}_e)$  changes when the field passes through the twin boundary, and the magnitude of the asymmetry is in good agreement with the experimentally quoted  $\lambda_J/L$  values. Note that the asymmetry is large for the  $\theta = \pi/4$  and small for  $\theta = -\pi/4$  (in fact it appears to vanish between  $\theta = -\pi/4$  and  $\theta = -\pi/3$ ) as was the case for the  $0 - 0$  junction. This agreement between experiment and theory gives further support to the claim that the  $s$ -wave component in the YBCO superconductor changes sign as the twin boundary is crossed. These results are for a 30 by 30 system and studies for the 1D system show that increasing the system size does not change the qualitative behavior of the  $I_c(\mathbf{H}_e)$  patterns but does increase the size of the critical currents and also moves the minima in the  $I_c(\mathbf{H}_e)$  patterns to-

wards zero field. This explanation for the experimental results has the consequence that  $I_c(\mathbf{H}_e) = -I_c(-\mathbf{H}_e)$  as follows from the time reversal symmetry of the junction. A deviation from this equality implies that time reversal symmetry is broken in the junction. It is also of interest to study experimentally the geometry G1 since some qualitative differences in the  $I_c(\mathbf{H}_e)$  patterns between the two geometries are expected to arise. For example in geometry G1 the asymmetry should vanish for symmetric  $0 - \pi$  junctions and for asymmetric junctions as  $h_x^e$  is reversed  $I_c(\mathbf{H}_e) - I_c(-\mathbf{H}_e)$  should be the same due to Eq. 9 (in contrast to changing sign as it does for geometry G2).

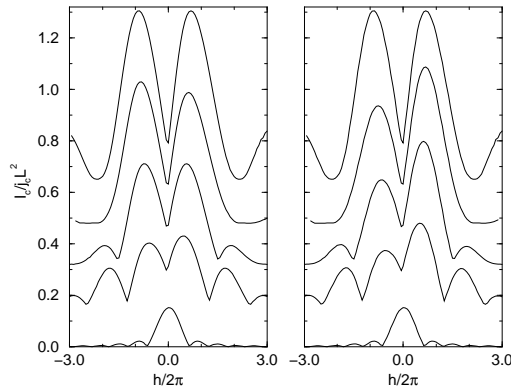


FIG. 3.  $I_c(\mathbf{H}_e)/j_c L^2$  for geometry G2, a symmetric  $0 - \pi$  junction, and  $\lambda_J/L = 0.5$ . From top to bottom correspond to  $\theta = 0, \pm\pi/6, \pm\pi/4, \pm\pi/3, \pi/2$  where positive (negative)  $\theta$  is on the right (left) side. Successive plots have been offset by 0.16.

In conclusion we have shown that parity breaking in time reversal invariant Josephson junctions lead to an asymmetry in the critical current as the magnetic field is reversed. A detailed examination of the magnetic diffraction patterns of  $0 - \pi$  junctions has shown that self-fields account well for unexplained features observed in single twin boundary junctions. Experimental tests have been proposed to further examine this theory.

We are grateful for the financial support of the Swiss Nationalfonds. In particular, M.S. was supported by a PROFIL-Fellowship and D.F.A. by the Zentrum for Theoretische Physik. D.F.A. acknowledges financial support from the Natural Sciences and Engineering Research Council of Canada. We also thank T.M. Rice and A. Schnidrig for many helpful discussions and B. Chen, A. Katz and J. Clarke for useful correspondence on their experiments.

- [1] D.A. Wollman, D.J. Van Harlingen, W.C. Lee, D.M. Ginsberg, and A.J. Leggett, Phys. Rev. Lett. **71**, 2134 (1993).
- [2] D.A. Brawner and H.R. Ott, Phys. Rev. B **50**, 6530 (1994).
- [3] A. Mathai, Y. Gim, R.C. Black, A. Amar, and F.C. Wellstood, Phys. Rev. Lett. **74**, 4523 (1995).
- [4] I. Iguchi and Z. Wen, Phys. Rev. B **49**, 12388 (1994).
- [5] D.A. Wollman, D.J. Van Harlingen, J. Giapintzakis, and D.M. Ginsberg, Phys. Rev. Lett. **74**, 797 (1995).
- [6] C.C. Tsuei, J.R. Kirtley, C.C. Chi, L.S. Yu-Jahnes, A. Gupta, T. Shaw, J.Z. Sun, and M.B. Ketchen, Phys. Rev. Lett. **73**, 593 (1994).
- [7] J. R. Kirtley, C.C. Tsuei, J.Z. Sun, C.C. Chi, L.S. Yu-James, A. Gupta, M. Rupp, and M.B. Ketchen, Nature **373**, 225 (1995).
- [8] J.H. Miller, Q.Y. Ying, Z.G. Zou, N.Q. Fan, J.H. Xu, M.F. Davis, and J.C. Wolfe, Phys. Rev. Lett. **74**, 2347 (1995).
- [9] A.G. Sun, D.A. Gajewski, M.B. Maple, and R.C. Dynes, Phys. Rev. Lett. **72**, 2267 (1994); A.S. Katz, A.G. Sun, R.C. Dynes, and K. Char, Appl. Phys. Lett. **66**, 105 (1995).
- [10] M. Sigrist, K. Kuboki, P.A. Lee, A.J. Millis, and T.M. Rice, Phys. Rev. B **53**, 2835 (1996).
- [11] M.B. Walker, Phys. Rev. B **53**, 5835 (1996); M.B. Walker and J. Luettmmer-Strathmann, Phys. Rev. B **54**, 588 (1996).
- [12] C. O'Donovan, D. Branch, J.P. Carbotte, and J.S. Preston, Phys. Rev. B **51**, 6588 (1995).
- [13] Q.P. Li, E.C. Koltenbah, and R. Joynt, Phys. Rev. B **48**, 437 (1993).
- [14] K.A. Kouznetsov, A.G. Sun, B. Chen, A.S. Katz, S.R. Bahcall, J. Clarke, R.C. Dynes, D.A. Gajewski, S.H. Han, M.B. Maple, J. Giapintzakis, J.-T. Kim, and D.M. Ginsberg, Phys. Rev. Lett. in press (preprint cond-mat/9705283).
- [15] D.F. Agterberg, M. Sigrist, A. Schnidrig, and T.M. Rice, preprint.
- [16] J. R. Kirtley, K. A. Moler, and D.J. Scalapino, Phys. Rev. B **54**, 886 (1997).
- [17] J.H. Xu, J.H. Miller, and C.S. Ting, Phys. Rev. B **51**, 11 958 (1995).
- [18] M. Tinkham, *Introduction to Superconductivity* (McGraw-Hill, New York, 1996).
- [19] C.S. Owen and D.J. Scalapino, Phys. Rev. **164**, 538 (1967).
- [20] A.J. Millis, Phys. Rev. B **49**, 15408 (1994).
- [21] M. Sigrist and K. Ueda, Rev. Mod. Phys. **63**, 239 (1991).